JYVÄSKYLÄN YLIOPISTO
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# Kantorovich formulation of Optimal Transport

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Optimal Transport Methods in Density Functional Theory
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# Kantorovich Duality

Let $X = \mathbb{R}^d$ (or $(X, d)$ be a Polish space) and $V_{ee} : X^N \to \mathbb{R} \cup \{+\infty\}$.
Given $\rho \in \mathcal{A} \subset \mathcal{P}(X)$, consider the following problem:

$$\mathcal{V}_{ee}[\rho] = \sup_{v \in \mathcal{F}} \left\{ N \int_X v(s) d\rho(s) : V_{ee}(x_1, \dots, x_N) - \sum_{i=1}^{N} v(x_i) \geq 0 \right\}.$$

Goal: Understand if there is a wide class of densities $\mathcal{A}$ and potentials $\mathcal{F} \subset L^1_\rho(X)$ such that a maximizer exists. Moreover

- What is the regularity maximizer $v_{opt}$ (e.g. Lipschitz)?
- Asymptotic behavoir of $v_{opt}(x_1)$ when $|x_1| \to +\infty$?
- Is $\mathcal{V}_{ee} : \mathcal{A} \to \mathbb{R} \cup \{+\infty\}$ continuous?
- $\mathcal{R}_N := \left\{ \rho : \mathbb{R}^3 \to \mathbb{R} : \rho \geq 0, \int_{\mathbb{R}^3} \rho = 1, \sqrt{\rho} \in H^1(\mathbb{R}^3) \right\} \subset \mathcal{A}$?

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# Kantorovich dual problem

The Kantorovich theory for multi-marginal optimal Transport for repulsive costs has been explored in the recent years.


W. Gangbo, V. Oliker. Existence of optimal maps in the reflector-type problems. ESAIM: COCV (2007).

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L. De Pascale. Optimal transport with Coulomb cost. Approximation and duality. ESAIM: Mathematical Modelling and Numerical Analysis (2015)

G. Buttazzo, T. Champion, L. De Pascale. Continuity and estimates for multimarginal optimal transportation problems with singular costs. Applied Mathematics & Optimization (2018).

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# Kantorovich Duality (idea)

Let $X = \mathbb{R}^d$ (or $(X, d)$ be a Polish space) and $\rho \in \mathcal{P}(X)$.

$$\begin{aligned}
\mathcal{V}_{ee}[\rho] &= \inf_{\gamma \in \Pi_N(\rho)} \int_{X^N} V_{ee}(x_1, \dots, x_N) d\gamma(x_1, \dots, x_N). \\
&= \inf_{\gamma \in \mathcal{M}(X^N)} \int_{X^N} V_{ee} d\gamma + \sup_{v \in C_b(X)} N \int_X v d\rho - \int_{X^N} \sum_{i=1}^N v(x_i) d\gamma \\
&= \sup_{v \in C_b(X)} N \int_X v d\rho + \inf_{\gamma \in \mathcal{M}(X^N)} \int_{X^N} \left( V_{ee}(x_1, \dots, x_N) - \sum_{i=1}^N v(x_i) \right) d\gamma \\
&= \sup_{v \in C_b(X)} \left\{ N \int_X v d\rho : v \in C_b(X), V_{ee}(x_1, \dots, x_N) - \sum_{i=1}^N v(x_i) \geq 0 \right\}
\end{aligned}$$

- Riesz-Markov-Kakutani representation theorem: duality between $\mathcal{M}(X^N)$ and $C_b(X)$.
- Fenchel-Rockafellar Theorem.

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# Monge-Kantorovich formulation

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- $\gamma \in \Pi_N(\rho)$: $\gamma \in \mathcal{P}(X^N)$ having all marginals equal to $\rho$.
- $V_{ee} : X^N \to \mathbb{R} \cup \{+\infty\}$ is a lower semi-continuous cost function.

$$V_{ee}(x_1, \dots, x_N) = \sum_{1 \le i < j \le N} w(d(x_i, x_j)), \quad w : [0, +\infty[ \to \mathbb{R} \cup \{+\infty\}$$

$w|_{]0,+\infty[}$ is a continuous, decreasing

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$$\mathcal{A} = \left\{ \rho \in \mathcal{P}(X) \quad : \quad \begin{array}{c} \lim_{r\to 0} \sup_{x\in X} \rho(B(x,r)) < \frac{1}{N(N-1)^2} \text{ and} \\ \exists o \in X, r_0 > 0 \text{ s.t. } \int_{X\setminus B(o,r_0)} w\left(2d(x,o)\right) \, d\rho(x) > -\infty \end{array} \right\}$$

THEOREM[1]

Let $(X,d)$ be a Polish space. Suppose $\rho \in \mathcal{A}$ and $V_{ee}$ as before. Then the following holds:

$$\min_{\gamma\in\Pi_N(\rho)} \int_{X^N} V_{ee} d\gamma = \max_{v\in L^1_\rho(X)} \left\{ \int_X v(x) d\rho(x) : V_{ee}(x_1,\dots,x_N) - \sum_{i=1}^N v(x_i) \geq 0 \right\}$$

Moreover,

$$V_{ee}(x_1,\dots,x_N) - \sum_{j=1}^N v(x_j) = 0, \quad \gamma - \text{almost every } (x_1,\dots,x_N) \in X^N$$

[1] H. G. KELLERER ($V_{ee} \leq \sum_{i=1}^N a_i$), $a_i \in L^1(\rho)$ (1984)
G. BUTTAZZO, T. CHAMPION, L. DE PASCALE (BOUNDED FROM BELOW CASE)
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## Paola Gori-Giorgi's remark:

For simplicity consider $X = \mathbb{R}^d$ and $V_{ee}(x_1, \dots, x_N)$ be the Coulomb cost

$$V_{ee}(x_1, \dots, x_N) = \sum_{1 \le i < j \le N} \frac{1}{|x_j - x_i|},$$

By applying $\nabla_{x_i}$, we have

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$$\nabla v(x_i) = -\sum_{i=1}^{N} \frac{x_j - x_i}{|x_j - x_i|^3}, \quad \gamma - \text{ almost every } (x_1, \dots, x_N) \in (\mathbb{R}^d)^N.$$

Now assume there is a SCE/Monge type minimizer for $\mathcal{V}_{ee}[\rho]$[2] then

$$\nabla v(x_i) = -\sum_{i=1}^{N} \frac{T_j(x_1) - T_i(x_1)}{|T_j(x_1) - T_i(x_1)|^3}, \quad x_1 \in X = \mathbb{R}^d.$$

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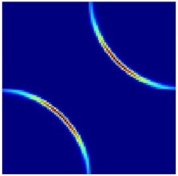
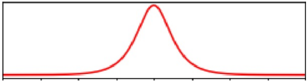
# Regularity of Kantorovich potentials

1ST INGREDIENT:

Let $\gamma \in \text{argmin}_{\gamma \in \Pi_N(\rho)} \int_{X^N} V_{ee} d\gamma$. Then there exists a $\alpha > 0$ such that

$$\text{spt}(\gamma) \subset X^N \setminus D_\alpha, \quad D_\alpha := \left\{ x = (x_1, \dots, x_N) \in X^N : \|x_i - x_j\| < \alpha \right\}.$$





2ND INGREDIENT:

$$v(x_1) = \inf \left\{ V_{ee}(x_1, \dots, x_N) - \sum_{j=2}^{N} v(x_j) \;\middle|\; (x_2, \dots, x_N) \in X^{N-1} \right\}, \quad \rho\text{−a.e. } x_1 \in X$$

PROPOSITION: Assume additionally that $V_{ee}$ is Lipschitz outside the singular set $D_\alpha$. Then, there exists a Kantorovich potential $u$ in the dual problem that is bounded, Lipschitz and semi-concave ($\nabla^2 u \geq \lambda Id, \lambda > 0$ $\rho$-a.e.).

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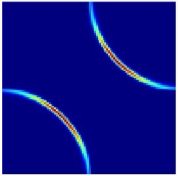

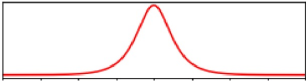

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# Continuity results

THEOREM[3]: Assume $\rho \in \mathcal{A}$. Then

(i) [Bounded case] If $V_{ee}$ is lower semi-continuous and bounded then $\mathcal{V}_{ee}[\rho]$ is $L^1$-Lipschitz in $\mathcal{A}$ with respect to the strong topology on $\mathcal{P}(X)$.

$$|\mathcal{V}_{ee}[\rho_1] - \mathcal{V}_{ee}[\rho_2]| \leq C\|\rho_1 - \rho_2\|_1.$$

If $V_{ee}$ is Lipschitz outside $D_\alpha$ then $\mathcal{V}_{ee}$ is $W_1-$ Lipschitz with respect to the weak*-topology.

(ii) [Unbounded case] $V_{ee}$ is Lipschitz outside the singular set $D_\alpha$, then $\mathcal{V}_{ee}[\rho]$ is continuous with respect to the weak*-topology on $\mathcal{P}(X)$.

[3] G. Buttazzo, T. Champion, L. De Pascale, AG, A. Kausamo, T. Rajala, M. Colombo, S. Di Marino, F. Stra

# Quantum analog[4]

$X = \mathbb{R}^3$. For simplicity, let consider the Coulomb case.

$$\mathcal{E}_\hbar[\rho] = \min_{\Gamma=\Gamma^*\geq 0, Tr(\Gamma)=1, \rho_\Gamma=\rho} \mathrm{Tr}\left(-\hbar^2 \sum_{i=1}^N \Delta_{x_i} + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|}\right)\Gamma$$

- $\rho \geq 0$ is a density such that $\int_{\mathbb{R}^3} \rho dx = 1$ and $\sqrt{\rho} \in H^1(\mathbb{R}^3)$.
- $\Gamma$ is an operator acting on the fermionic space $\bigwedge_{i=1}^N L^2(\mathbb{R}^3)$.
- $\mathcal{E}_\hbar[\rho]$ was introduced by Levy (1979) with the additional constraint that $\Gamma = |\phi\rangle\langle\phi|$ (pure state).

[4] E.H. Lieb, Density functionals for Coulomb systems. Int. J. Quant. Chem., 24 (1983)
M. Lewin, Semi-classical limit of the Levy-Lieb functional. Comptes Rendus Mathematique (2018).

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$$= \sup\left\{ N\int v_\hbar(x)\rho(x)dx : \begin{array}{r} v_\hbar \in L^{3/2}(\mathbb{R}^3,\mathbb{R}) + L^\infty(\mathbb{R}^3,\mathbb{R}), \\ -\hbar^2\sum_{i=1}^N \Delta_{x_i} + \sum_{1\leq i<j\leq N}\frac{1}{|x_i-x_j|} + \sum_{i=1}^N v_\hbar(x_i) \geq 0 \end{array} \right\}$$

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$X = \mathbb{R}^d$

THEOREM (S. DI MARINO, AG): Let $\rho \in \mathcal{A}$ be an absolutely continuous measure such that $\mathrm{spt}(\rho) = \mathbb{R}^d$. Consider $V_{ee}$ as before and $u$ a bounded optimal potential for $\rho$. Then,

(i) $\exists\ \beta_u < 0$ such that $u(x) \geq \beta_u$ and $\lim_{|x|\to\infty} u(x) = \beta_u$.

(ii) We have

$$\lim_{|x|\to\infty} \frac{(u(x) - \beta_u)}{w(x)} = N - 1.$$

(iii) Assume that $d = 3$, $w(|x|) = |x|^{-1}$. There exist a non-negative locally finite measure $\mu \in \mathcal{M}(\mathbb{R}^3)$ such that $\mu(\mathbb{R}^3) = N - 1$ and

$$-\Delta u = \mu$$

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$$u(x) = \beta_u + \int_{\mathbb{R}^3} w(x-y)d\mu(y).$$